From multidimensional replica-exchange method to multidimensional multicanonical algorithm and simulated tempering

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We discuss multidimensional generalizations of multicanonical algorithm, simulated tempering, and replica-exchange method. We generalize the original potential-energy function E_0 by adding any physical quantity V of interest as a new energy term with a coupling constant λ. We then perform a multidimensional multicanonical simulation where a random walk in E_0 and V spaces is realized. We can alternately perform a multidimensional simulated-tempering simulation where a random walk in temperature T and parameter λ is realized. The results of the multidimensional replica-exchange simulations can be used to determine the weight factors for these multidimensional multicanonical and simulated-tempering simulations.

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Monte Carlo (MC) and molecular dynamics (MD) simulations of frustrated systems such as spin glass and biomolecular systems are very difficult because their free-energy landscapes are rugged. In order to overcome this difficulty, *generalized-ensemble algorithms* have often been employed (for reviews, see, for instance, Refs. [1–4]). Generalized-ensemble algorithms are based on artificial non-Boltzmann weight factors so that random walks in potential-energy space and other variable space may be realized. Once an optimal weight factor is found, one makes a single long production run. From the results of this production run, one can reconstruct canonical realistic ensembles for a wide range of temperature and other parameter values by the single-histogram [5] or multiple-histogram [6] reweighting techniques. *Multicanonical algorithm* (MUCA) [7,8], *simulated tempering* (ST) [9,10], and *replica-exchange method* (REM) [11] are three of the most widely used generalized-ensemble algorithms. A powerful method closely related to MUCA is *Wang-Landau method* [12]. ST is also referred to as the *method of expanded ensemble* [9]. REM is also referred to as *parallel tempering* [13]. A similar method to REM was also developed in Ref. [14]. A general formulation for the multidimensional REM is already given [15]. In this paper, we present general formulations for multidimensional extensions of MUCA and ST, where we use a short multidimensional REM simulation to determine the multidimensional MUCA and ST weight factors.

Let us consider the following generalized potential-energy function of a system in state x:

$$E_{\boldsymbol{\lambda}}(x) = E_0(x) + \sum_{\ell=1}^{L} \lambda^{(\ell)} V_\ell(x). \tag{1}$$

Here, there are $L+1$ energy terms, $E_0(x)$ and $V_\ell(x)$ $(\ell=1,\ldots,L)$, and $\lambda^{(\ell)}$ are the corresponding coupling constants for $V_\ell(x)$ [we collectively write $\boldsymbol{\lambda}=(\lambda^{(1)},\ldots,\lambda^{(L)})$]. The partition function of the system at fixed temperature T and parameters $\boldsymbol{\lambda}$ is then given by

$$\begin{aligned} Z(T,\boldsymbol{\lambda}) &= \int dx \exp[-\beta E_{\boldsymbol{\lambda}}(x)] \\ &= \int dE_0 dV_1 \cdots dV_L n(E_0,V_1,\ldots,V_L)\exp(-\beta E_{\boldsymbol{\lambda}}), \end{aligned} \tag{2}$$

where $\beta=1/k_BT$, k_B is the Boltzmann constant, and $n(E_0,V_1,\ldots,V_L)$ is the multidimensional density of states. Here, the integral is replaced by a summation when x is discrete.

The expression in Eq. (1) is often used in simulations. For instance, in simulations of spin systems, $E_0(x)$ and $V_1(x)$ (here, $L=1$ and $x=\{S_1,S_2,\ldots\}$ stand for spins) can be, respectively, considered as the zero-field and the magnetization terms coupled with the external field $\lambda^{(1)}$. (For Ising model, $E_0=-J\Sigma_{\langle i,j\rangle}S_iS_j$, $V_1=-\Sigma_iS_i$, and $\lambda^{(1)}=h$, i.e., external magnetic field.) In umbrella sampling [16] in molecular simulations, $E_0(x)$ and $V_\ell(x)$ can be taken as the original potential and the "biasing" umbrella potential energies, respectively, with the coupling parameter $\lambda^{(\ell)}$ (here, $x=\{\boldsymbol{q}_1,\ldots,\boldsymbol{q}_N\}$, where $\boldsymbol{q}_i$ are the coordinate vectors of the ith particle and N is the total number of particles). For the molecular simulations in the isobaric-isothermal ensemble, $E_0(x)$ and $V_1(x)$ (here, $L=1$) can be, respectively, considered as the potential energy U and the volume $\mathcal{V}$ coupled with the pressure $\mathcal{P}$. (Namely, we have $x=\{\boldsymbol{q}_1,\ldots,\boldsymbol{q}_N,\mathcal{V}\}$, $E_0=U$, $V_1=\mathcal{V}$, and $\lambda^{(1)}=\mathcal{P}$, i.e., $E_{\boldsymbol{\lambda}}$ is the enthalpy without the kinetic-energy contributions.) For simulations in the grand canonical ensemble with N particles, we have $x=\{\boldsymbol{q}_1,\ldots,\boldsymbol{q}_N,N\}$, and $E_0(x)$ and $V_1(x)$ (here, $L=1$) can be, respectively, considered as the potential energy U and the total number of particles N coupled with the chemical potential μ. (Namely, we have $E_0=U$, $V_1=N$, and $\lambda^{(1)}=-\mu$.) We remark that generalized-ensemble algorithms in various ensembles are also discussed in Refs. [17,18].

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Moreover, we can introduce any physical quantity of interest (or its function) as the additional potential-energy term V_ℓ. For instance, V_ℓ can be an overlap with a reference configuration in spin glass systems, an end-to-end distance, and a radius of gyration in molecular systems, etc. In such a case, we have to carefully choose the range of $\lambda^{(\ell)}$ values so that the new energy term $\lambda^{(\ell)}V_\ell$ will have roughly the same order of magnitude as the original energy term E_0.

We first describe the multidimensional MUCA simulation which realizes a random walk in the $(L+1)$-dimensional space of $E_0(x)$ and $V_\ell(x)$ $(\ell=1,\ldots,L)$. In the multidimensional MUCA ensemble, each state is weighted by the MUCA weight factor $W_{\mathrm{MU}}(E_0,V_1,\ldots,V_L)$ so that a uniform energy distribution of E_0, $V_1,\ldots$, and V_L may be obtained:

$$P_{\mathrm{MU}}(E_0,V_1,\ldots,V_L) \propto n(E_0,V_1,\ldots,V_L)W_{\mathrm{MU}}(E_0,V_1,\ldots,V_L) \equiv \text{const}, \tag{3}$$

where $n(E_0,V_1,\ldots,V_L)$ is the multidimensional density of states. From this equation, we obtain

$$W_{\mathrm{MU}}(E_0,V_1,\ldots,V_L) \propto \frac{1}{n(E_0,V_1,\ldots,V_L)} \equiv \exp[-\beta_a E_{\mathrm{MU}}(E_0,V_1,\ldots,V_L)], \tag{4}$$

where in the second line we have introduced an arbitrary reference temperature, $T_a=1/k_B\beta_a$, and wrote the weight factor in the Boltzmann-type form. Here, the "*multicanonical potential energy*" is defined by

$$E_{\mathrm{MU}}(E_0,V_1,\ldots,V_L) \equiv k_B T_a \ln n(E_0,V_1,\ldots,V_L). \tag{5}$$

The multidimensional MUCA MC simulation can be performed with the following Metropolis transition probability from state x with energy $E_{\boldsymbol{\lambda}}=E_0+\sum_{\ell=1}^{L}\lambda^{(\ell)}V_\ell$ to state x' with energy $E_{\boldsymbol{\lambda}'}=E_0'+\sum_{\ell=1}^{L}\lambda^{(\ell)}V_\ell'$:

$$w(x\to x') = \min\left(1,\frac{W_{\mathrm{MU}}(E_0',V_1',\ldots,V_L')}{W_{\mathrm{MU}}(E_0,V_1,\ldots,V_L)}\right) = \min\left(1,\frac{n(E_0,V_1,\ldots,V_L)}{n(E_0',V_1',\ldots,V_L')}\right). \tag{6}$$

An MD algorithm in the multidimensional MUCA ensemble also naturally follows from Eq. (4), in which a regular constant-temperature MD simulation (with $T=T_a$) is performed by replacing the total potential energy $E_{\boldsymbol{\lambda}}$ by the multicanonical potential energy E_{MU} in Newton's equations for the kth particle $(k=1,\ldots,N)$ (see Refs. [19,20] for one-dimensional version):

$$\dot{\boldsymbol{p}}_k = -\frac{\partial E_{\mathrm{MU}}(E_0,V_1,\ldots,V_L)}{\partial \boldsymbol{q}_k}. \tag{7}$$

Second, we consider a multidimensional ST simulation which realizes a random walk both in temperature T and in parameters $\boldsymbol{\lambda}$. The parameter set $\boldsymbol{\Lambda}=(T,\boldsymbol{\lambda}) \equiv (T,\lambda^{(1)},\ldots,\lambda^{(L)})$ becomes dynamical variables, and both the configuration and the parameter set are updated during the simulation with a weight factor:

$$W_{\mathrm{ST}}(\boldsymbol{\Lambda}) \equiv \exp[-\beta E_{\boldsymbol{\lambda}} + f(\boldsymbol{\Lambda})], \tag{8}$$

where the function $f(\boldsymbol{\Lambda})=f(T,\boldsymbol{\lambda})$ is chosen so that the probability distribution of $\boldsymbol{\Lambda}$ is flat:

$$P_{\mathrm{ST}}(\boldsymbol{\Lambda}) \propto \int dE_0 dV_1 \cdots dV_L n(E_0,V_1,\ldots,V_L) \times \exp[-\beta E_{\boldsymbol{\lambda}} + f(\boldsymbol{\Lambda})] \equiv \text{const}. \tag{9}$$

This means that $f(\boldsymbol{\Lambda})$ is the dimensionless ("Helmholtz") free energy:

$$\exp[-f(\boldsymbol{\Lambda})] \propto \int dE_0 dV_1 \cdots dV_L n(E_0,V_1,\ldots,V_L) \times \exp(-\beta E_{\boldsymbol{\lambda}}). \tag{10}$$

In the numerical work we discretize the parameter set $\boldsymbol{\Lambda}$ in $M(=M_0\times M_1\times\cdots\times M_L)$ different values: $\boldsymbol{\Lambda}_m \equiv (T_{m_0},\boldsymbol{\lambda}_m) \equiv (T_{m_0},\lambda_{m_1}^{(1)},\ldots,\lambda_{m_L}^{(L)})$, where $m_0=1,\ldots,M_0$, $m_\ell=1,\ldots,M_\ell$ $(\ell=1,\ldots,L)$. Without loss of generality we can order the parameters so that $T_1<T_2<\cdots<T_{M_0}$ and $\lambda_1^{(\ell)}<\lambda_2^{(\ell)}<\cdots<\lambda_{M_\ell}^{(\ell)}$ (for each $\ell=1,\ldots,L$). The free energy f is now written as $f_{m_0,m_1,\ldots,m_L}=f(T_{m_0},\lambda_{m_1}^{(1)},\ldots,\lambda_{m_L}^{(L)})$.

Once the initial configuration and the initial parameter set are chosen, the multidimensional ST is realized by alternately performing the following two steps: (1) A canonical MC or MD simulation at the fixed parameter set $\boldsymbol{\Lambda}_m=(T_{m_0},\boldsymbol{\lambda}_m)=(T_{m_0},\lambda_{m_1}^{(1)},\ldots,\lambda_{m_L}^{(L)})$ is carried out for a certain steps with the weight factor $\exp(-\beta_{m_0}E_{\boldsymbol{\lambda}})$. (2) We update the parameter set $\boldsymbol{\Lambda}_m$ to a new parameter set $\boldsymbol{\Lambda}_{m\pm1}$ in which one of the parameters in $\boldsymbol{\Lambda}_m$ is changed to a neighboring value with the configuration and the other parameters fixed. The transition probability of this parameter-updating process is given by the following Metropolis criterion:

$$w(\boldsymbol{\Lambda}_m\to\boldsymbol{\Lambda}_{m\pm1}) = \min\left(1,\frac{W_{\mathrm{ST}}(\boldsymbol{\Lambda}_{m\pm1})}{W_{\mathrm{ST}}(\boldsymbol{\Lambda}_m)}\right) = \min[1,\exp(-\Delta)]. \tag{11}$$

Here, there are two possibilities for $\boldsymbol{\Lambda}_{m\pm1}$, and we have $\boldsymbol{\Lambda}_{m\pm1}=(T_{m_0\pm1},\ldots,\lambda_{m_\ell}^{(\ell)},\ldots)$ with

$$\Delta = (\beta_{m_0\pm1}-\beta_{m_0})E_{\boldsymbol{\lambda}_m} - (f_{m_0\pm1,m_1,\ldots,m_L} - f_{m_0,m_1,\ldots,m_L}), \tag{12}$$

for T update, and $\boldsymbol{\Lambda}_{m\pm1}=(T_{m_0},\ldots,\lambda_{m_\ell\pm1}^{(\ell)},\ldots)$ with

$$\Delta = \beta_{m_0}(\lambda_{m_\ell\pm1}^{(\ell)}-\lambda_{m_\ell}^{(\ell)})V_\ell - (f_{m_0,\ldots,m_\ell\pm1,\ldots} - f_{m_0,\ldots,m_\ell,\ldots}), \tag{13}$$

for $\lambda^{(\ell)}$ update (for one of $\ell=1,\ldots,L$).

We remark that the random walk in E_0 and in V_ℓ for the MUCA simulation corresponds to that in β and in $\beta\lambda^{(\ell)}$ for the ST simulation: $E_0\leftrightarrow\beta$ and $V_\ell\leftrightarrow\beta\lambda^{(\ell)}$, $(\ell=1,\ldots,L)$. They are in conjugate relation.

We can perform the multidimensional MUCA and ST simulations when we have optimal weight factors. However, we do not know these MUCA and ST weight factors *a priori* and need to estimate them. In previous works [21–23], we

developed powerful methods to determine MUCA and ST weight factors by a short REM simulation and the multiple-histogram reweighting techniques in the one-dimensional case. Here, we generalize the methods to multidimensional versions (see also Refs. [3,4]).

We use a short multidimensional REM simulation [15] to determine the multidimensional MUCA and ST weight factors. The system for the multidimensional REM consists of M noninteracting replicas of the original system in the "canonical ensemble" with $M(=M_0\times M_1\times\ldots\times M_L)$ different parameter sets $\mathbf{\Lambda}_m$ $(m=1,\ldots,M)$. Because the replicas are noninteracting, the weight factor is given by the product of Boltzmann factor for each replica:

$$W_{\mathrm{MREM}} \equiv \prod_{m_0=1}^{M_0}\prod_{m_1=1}^{M_1}\cdots\prod_{m_L=1}^{M_L}\exp(-\beta_{m_0}E_{\boldsymbol{\lambda}_m}). \tag{14}$$

REM closely follows the ST procedures described above. In step 1, a "canonical" MC or MD simulation at the fixed parameter set is carried out for each replica simultaneously and independently for a certain MC or MD steps. In step 2, we exchange a pair of replicas i and j which are at the parameter sets $\mathbf{\Lambda}_m$ and $\mathbf{\Lambda}_{m+1}$, respectively. The transition probability for this replica-exchange process is given by

$$w(\mathbf{\Lambda}_m \leftrightarrow \mathbf{\Lambda}_{m+1}) = \min[1,\exp(-\Delta)], \tag{15}$$

where we have

$$\Delta = (\beta_{m_0}-\beta_{m_0+1})[E_{\boldsymbol{\lambda}_m}(q^{[j]})-E_{\boldsymbol{\lambda}_m}(q^{[i]})], \tag{16}$$

for T exchange, and

$$\Delta = \beta_{m_0}(\lambda^{(\ell)}_{m_\ell}-\lambda^{(\ell)}_{m_\ell+1})[V_\ell(q^{[j]})-V_\ell(q^{[i]})], \tag{17}$$

for $\lambda^{(\ell)}$ exchange (for one of $\ell=1,\ldots,L$). Here, $q^{[i]}$ and $q^{[j]}$ stand for configuration variables for replicas i and j, respectively, before the replica exchange. Usually, $M_0/2$ or $M_\ell/2$ pairs of replicas corresponding to neighboring T or $\lambda^{(\ell)}$ are simultaneously exchanged, and the pairing is alternated between the two possible choices, i.e., $(T_1,T_2),(T_3,T_4),\ldots$ and $(T_2,T_3),(T_4,T_5),\ldots$, or $(\lambda_1^{(\ell)},\lambda_2^{(\ell)}),(\lambda_3^{(\ell)},\lambda_4^{(\ell)}),\ldots$ and $(\lambda_2^{(\ell)},\lambda_3^{(\ell)}),(\lambda_4^{(\ell)},\lambda_5^{(\ell)}),\ldots$, respectively.

To obtain the canonical distributions, the multiple-histogram reweighting techniques [6] are particularly useful. Suppose we have made a single run of the multidimensional REM simulation with $M(=M_0\times M_1\times\cdots\times M_L)$ replicas that correspond to M different parameter sets $\mathbf{\Lambda}_m$ $(m=1,\ldots,M)$. Let $N_{m_0,m_1,\ldots,m_L}(E_0,V_1,\ldots,V_L)$ and $n_{m_0,m_1,\ldots,m_L}$ be, respectively, the $(L+1)$-dimensional potential-energy histogram and the total number of samples obtained for the mth parameter set $\mathbf{\Lambda}_m=(T_{m_0},\lambda^{(1)}_{m_1},\ldots,\lambda^{(L)}_{m_L})$. The multiple-histogram reweighting equations are given by [6]

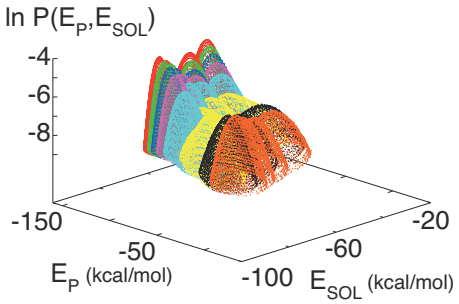

FIG. 1. (Color) Canonical distributions $P(E_P,E_{\mathrm{SOL}})$ with the 32 possible parameter sets (T_{m_0},λ_{m_1}), which were obtained by the short two-dimensional REM simulation.

$$n(E_0,V_1,\ldots,V_L) = \frac{\sum_{m_0,m_1,\ldots,m_L} N_{m_0,m_1,\ldots,m_L}(E_0,V_1,\ldots,V_L)}{\sum_{m_0,m_1,\ldots,m_L} n_{m_0,m_1,\ldots,m_L}\exp(f_{m_0,m_1,\ldots,m_L}-\beta_{m_0}E_{\boldsymbol{\lambda}_m})}, \tag{18}$$

and

$$\exp(-f_{m_0,m_1,\ldots,m_L}) = \sum_{E_0,V_1,\ldots,V_L} n(E_0,V_1,\ldots,V_L)\times\exp(-\beta_{m_0}E_{\boldsymbol{\lambda}_m}). \tag{19}$$

The density of states $n(E_0,V_1,\ldots,V_L)$ and the dimensionless free energy $f_{m_0,m_1,\ldots,m_L}$ are obtained by solving Eqs. (18) and (19) self-consistently by iteration. The canonical probability distribution at any temperature $T=1/k_B\beta$ with any potential-energy parameter value $\boldsymbol{\lambda}$ is then given by $P(E_0,V_1,\ldots,V_L)=n(E_0,V_1,\ldots,V_L)\exp(-\beta E_{\boldsymbol{\lambda}})$.

Finally, the weight factors for multidimensional MUCA [see Eq. (4)] and multidimensional ST [see Eqs. (8) and (10)] are obtained from the generalized density of states $n(E_0,V_1,\ldots,V_L)$ and the dimensionless free energy $f_{m_0,m_1,\ldots,m_L}$, respectively.

As an example of the applications of the present formulations, we now present the results of a two-dimensional ST simulation. The system is a bimolecular system, namely, a 17-residue helical peptide fragment of ribonuclease T_1, which was studied in Ref. [22]. We set $E_\lambda=E_P+\lambda E_{\mathrm{SOL}}$, where we have $L=1$ in Eq. (1), and $E_0=E_P$ is the conformational energy of the biomolecule and $V_1=E_{\mathrm{SOL}}$ is the solvent energy. The simulations were started from randomly generated conformations. We prepared eight temperatures which are distributed exponentially between $T_1=300$ K and $T_8=700$ K (i.e., 300.00, 338.60, 382.17, 431.36, 486.85, 549.49, 620.20, and 700.00 K) and four equally spaced λ values ranging from zero to one (i.e., $\lambda_1=0$, $\lambda_2=1/3$, $\lambda_3=2/3$, and $\lambda_4=1$). The total number of replicas is then 32 $(=8\times4)$.

In Fig. 1, the canonical probability distributions at 32 conditions obtained from the two-dimensional REM simulation are shown. For an optimal performance of the REM simulation, there should be enough overlaps between all pairs of

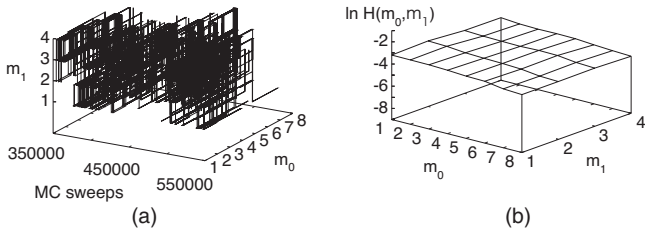

FIG. 2. (a) Time series and (b) histogram $H(m_0,m_1)$ of the parameter labels m_0 and m_1 for (T_{m_0},λ_{m_1}), which were obtained by the two-dimensional ST simulation.

neighboring distributions, which will lead to sufficiently uniform and large acceptance ratios of replica exchange. We see in Fig. 1 that there are indeed ample overlaps between the neighboring distributions.

Using the results of this multidimensional REM simulation, we obtained the two-dimensional ST parameters f_{m_0,m_1} $(m_0=1,\ldots,8;\ m_1=1,\ldots,4)$ by the multiple-histogram reweighting techniques [see Eqs. (8), (18), and (19)], and performed a two-dimensional ST simulation.

The time series of labels of temperature T and parameter λ is shown in Fig. 2(a). The random walk in both T and λ spaces was indeed realized. The histogram of labels of T and λ is shown in Fig. 2(b). We did get an expected flat histogram in T and λ. Hence, the two-dimensional ST simulation was successfully performed.

In this paper, we discussed multidimensional generalizations of MUCA, ST, and REM. While the multidimensional REM simulation can be easily performed because no weight factor determination is necessary, the required number of replicas can be quite large and computationally demanding. We thus prefer to use the multidimensional MUCA or ST, where only a single replica is simulated, instead of REM. However, it is very difficult to obtain optimal weight factors for the multidimensional MUCA and ST. Here, we have proposed a powerful method to determine these weight factors. Namely, we first perform a short multidimensional REM simulation and use the multiple-histogram reweighting techniques. The multidimensional generalized-ensemble algorithms that were presented in the present paper will be very useful for Monte Carlo and molecular-dynamics simulations of complex systems such as spin glass and biomolecular systems.

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